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## Hierarchical multiscale method for coupled mechano-electronic modeling of semiconducting nanomaterials

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### ABSTRACT

This discussion presents a hierarchical multiscale framework that furnishes a two-level statement of the problem and facilitates simultaneous resolution of quasi-continuum and atomistic length scales in a unified manner. Interatomic interactions are incorporated in the method through a set of analytical equations that contain nanoscale-based material moduli. These material moduli are defined via internal variables that are functions of the local atomic configuration parameters. Point defects like vacancy defects in nanomaterials perturb the atomic structure locally and generate localized force fields. Formation energy of vacancy is evaluated via interatomic potentials and minimization of this energy leads to nanoscale force field around defects which is then employed in the multiscale method to solve for the localized displacements in the vicinity of vacancies and defects. Electronic structure of the deforming semiconducting material is modeled by nonlinear Schrödinger wave equation that is embedded with a nonlocal potential as well as the nonlinear Hartree and exchange correlation potentials, solved in a self-consistent fashion. Accuracy and convergence properties of the method are assessed through test cases and the superior performance of higher-order B-splines and NURBS basis functions when compared with the corresponding Lagrange basis functions is highlighted. Self-consistent solutions for materials like Silicon (Si), Gallium Arsenide (GaAs), and Graphene are shown, and an application of the coupled solution method to strained nanomaterials is presented.

### REFERENCES

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